Synopsis for Ph.D. Programme

Title of the Research:

SOME STUDIES ON WAVELET-BASED NUMERICAL TECHNIQUES FOR PERIDYNAMIC PROBLEMS

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The peridynamic (PD) model proposed by Silling (Silling, 2000) is an integral-type nonlocal continuum model of materials which provides an alternative set up to classical continuum mechanics based on partial differential equations. Peridynamics was developed as a reformulation of elasticity theory for handling discontinuities in solid mechanics. Since then it has been applied to a variety of problems including damage, failure and multiscale material modeling (Silling et al., 2003; Silling and Askari, 2005; Weckner and Abeyaratne, 2005; Emmrich and Weckner, 2007; Weckner et al.,2007; Askari et al., 2008; Kilic and Madenci, 2009; Weckner et al., 2009). In the PD modeling of continuum mechanics each material point is connected (via PD bonds) with nodes in a certain region around it and not only with its nearest neighbours. This method is particularly well suited for dealing with cracks and damages in solid mechanics, especially in situations where the crack path is not known in advance. Peridynamics connects continuum mechanics and molecular dynamics within a single framework.

Peridynamics differs from other integral nonlocal methods in atleast two crucial aspects : (1) spatial derivatives are eliminated while other methods average infinitesimal stresses over a certain area and (2) the way damage and fractures are introduced in the method. As peridynamics avoids the explicit use of spatial derivatives, its effectiveness in modeling materials singularities has been observed in numerical simulations of crack nucleation and growth, fracture and failure of composites, polycrystals, and nanofiber networks.

Classical continuum mechanics has been applied to explain the behavior of structural bodies which remain continuous as they deform under external loads. However, the effectiveness of computational methods based on classical continuum mechanics, such as finite elements, in modeling material failure has lagged far behind their capabilities in traditional stress analysis. This difficulty arises because these methods solve the classical equations of continuum mechanics, which are a set of partial differential equations. These equations cannot be applied directly across discontinuities resulted from material damage and failure, as the required partial derivatives do not exist there. This mathematical breakdown result in great difficulties in attempting to model material failure directly and leads to special technique in fracture mechanics to treat discontinuities, such as cracks or pathological situation. These limitations become particularly inconvenient in the case of composite materials because it is very difficult to track individual defect, which grow in constituent materials, along interfaces, and between different layers, and moreover, interact with each other.

The PD theory does not suffer from the inapplicability when discontinuities are present and offers a unique capability to predict material failure. In the PD theory, the emergence and growth of discontinuous areas, such as fractures or cracks, are treated as just another form of deformation rather than as pathological cases.

The numerical model of PD theory has been successfully applied to damage analysis of metallic structures and nano-scale structures. Recently, its applications are extended to damage and failure analysis of composite materials. Within the context of PD-based nonlocal models, there have

been a variety of numerical methods implemented for their approximations including finite difference, finite element, quadrature, and particle-based methods.

In numerical analysis, classical discretization methods, such as finite differences, finite elements, spectral elements are powerful tools for solving differential equations. However, singularities and rapid changes often emerge in many phenomena, like stress concentration, elastoplasticity, shock wave and crack. Since small-scale features only exists in a small percentage of the solution domain, if one chooses a uniform numerical grid fine enough to resolve the small-scale characteristics, then the solutions to the equations will be over-resolved in the majority of the domain. One would like, ideally, to have a dense grid where small-scale structure exists and a sparse grid where the solution is only composed of large-scale features. It demands for the usage of non-uniform grids or moving elements to dynamically adapt to the changes in the solution. That is where wavelets play role.

Wavelet analysis is a new method called 'numerical microscope' in signal and image processing. It has the desirable advantages of various bases comprising multiresolution properties, which fulfill an enormous potential for solving differential/integral equations. The numerical analysis with wavelets received its first attention in the nineties of last century, since then researchers have shown growing interest in it.

In 1991, Beylkin and others (Beylkin et al., 1991) first carried out the study of numerical calculation based on wavelet. Daubechies wavelet (Daubechies, 1988) was used in calculation process. Subsequently, Jaffard (Jaffard, 1992) proved the superiority of solving elliptic partial differential equations by use of wavelet. Zweig (Zweig, 1997) found that the generalized wave equation, on which the continuous wavelet transform is based, can be used to understand phenomena related to the hearing process. Dahmen (Dahmen and Micchelli, 1993) and Chen (Chen and Temam, 1993) initiated related studies. These early literatures had a great influence and motivated the applications of wavelet in numerical calculation. During the past two decades, the theories of wavelet numerical methods have been developed in a variety of directions (K. Urban, 2002; A. Cohen, 2003; G.W. Pan 2003; G.P. Nason, 2008; S. Gopalakrishnan and M. Mitra, 2010). In summary, from the aspect of algorithm construction, the main wavelet-based numerical methods are categorized as follows :

- Wavelet weighted residual method (WWRM)
- Wavelet finite element method (WFEM)
- Wavelet boundary element (WBE)
- Wavelet meshless method (WMM)
- Other wavelet-based numerical methods

The underlying theory of wavelet-based numerical scheme is Multiresolution analysis (MRA) of function space. It comprises refinable functions and wavelets with compact support, is emerging field in pure and applied mathematics and it has applications in many areas of mathematical physics and engineering. This can be attributed due to its elegant role of mathematical microscopy in the analysis of smoothness or regularity of a function. The main advantages of a numerical method involving expansion of the unknown function in terms of refinable functions and wavelets compared to a classical method are that discretization of the domain involved is inbuilt in the technique due to compact support of the members in the basis and resulting matrix is sparse due to vanishing moments of the wavelets. The numerical scheme involving basis of MRA becomes comparatively stable and the related computational time is economic.

Our aim is to develop an efficient, reliable, computationally economic numerical scheme based on multiresolution analysis of function space for getting multiscale (approximate) solution of differential equations, integral equations, integro-differential equations, delay-differential equations, fractional differential equations etc. which often appear as the mathematical models in peridynamics and continuum mechanics at nano-scale. The possible steps of this study may be summarized as :

(i) Finding efficient orthonormal wavelet basis B_1 including their multiresolution properties (low- and high- pass boundary filters) within finite domain [a,b] in R.

(ii) Use of elements in B_1 to get basis B_2 (or B_3) for a domain D in R^2(or R^3).

(iii) Finding data (nodes and weights) of quadrature rule for integrals involving elements (scale functions / wavelets) in the basis B_i ,i=1,2,3 and any integrable function defined on D .

(iv) Regularization of singular functions / operators with the aid of wavelets.

(v) Multi-scale / multiresolution representation of operators (differential / integral / delay-differential / fractional differential operators etc.).

(vi) Transformation of data (initial, boundary conditions or constraints) in wavelet basis.

(vii) Reduction of equations involving differential / integral / integro-differential / delay-differential / fractional differential operators to algebraic equations for unknown coefficients of the expansion of unknown solution in wavelet basis, and their solution.

(viii) Estimation of error (a-posteriori) in approximate solution in terms of coefficients, as well as the analysis of computational complexity.

(ix) Application to some problems in peridynamics and nano-mechanics to check the efficiency and utility of this scheme.

(x) Development of ready to use (userfriendly) package (preferably incorporating CUDA or OPENCL programming languages for GPU) of the scheme so that it can be used by technical person efficiently.

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